

A TOY MODEL TEST OF A NEW ALGORITHM FOR BOZONIZATION OF FERMION DETERMINANTS

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Abstract

Different aspects of bozonization algorithm proposed in [5, 6] are tested by numerical simulations of a one dimensional toy model.

1 Introduction.

Computer simulations in lattice models with fermions meet serious difficulties due to grassmanian nature of fermionic variables. The method mainly used so far was based on the Hybrid Monte Carlo algorithm [1]. Considerable progress was achieved in this direction but with the present computer facilities it still does not allow efficient calculations in models with dynamical fermions.

An alternative approach was put forward by M.Lusher [2, 3], who proposed to calculate a fermion determinant replacing it by an infinite series of boson determinants. However at present the efficiency of this algorithm is comparable with the efficiency of Hybrid Monte Carlo method mainly due to the large autocorrelation time. (For a recent review of different approaches to the problem see [4]).

So at the moment the problem is still open and alternative approaches to bozonization should be investigated. In papers [5, 6] a representation of a D-dimensional fermion determinant as a path integral of a (D+1)-dimensional Hermitean bozonic action was proposed. This construction provides a new algorithm for numerical simulations of lattice QCD with dynamical quarks, although it is generally applicable to any model whose action is quadratic in Fermi fields and the matrix of quadratic form is positive definite. To study various technical aspects of a simulation procedure we carry out in the present paper a detailed study of a one dimensional toy model. In the original paper [5] bozonization procedure was based on the constrained bozonic effective action. Later it was observed [6] that using a freedom in the choice of effective bozonic action one can get rid off the constraints which seems to be more convenient for Monte-Carlo simulations. In this paper we use the unconstrained version.

2 Effective bozonic action.

Let us consider a D-dimensional lattice fermionic model with the action:

$$S_f = a^D \sum_x \bar{\psi}(x) (B^2 + m^2) \psi(x) \quad (1)$$

where x numerates the sites of a D-dimensional Euclidean hypercubic lattice, and B^2 is some positive bounded operator. (We shall assume also that the operator B is Hermitean, although it is not really necessary.)

We introduce (D+1)-dimensional bozonic fields $\phi(x, t)$ which have the same spinorial and internal structure as $\psi(x)$.

The extra coordinate t is defined on the one dimensional chain of the length L with the lattice spacing b :

$$L = Nb ; 0 \leq n < N \quad (2)$$

We assume that $b \parallel B \parallel \ll 1$.

The determinant of the operator $B^2 + m^2$ can be presented as the following bozonic path integral [5, 6]:

$$Det(B^2 + m^2) = \int e^{-S_f} D\bar{\psi} D\psi = \lim_{L \rightarrow \infty, b \rightarrow 0} \int e^{-S_b[\phi, \chi]} D\phi^* D\phi D\chi^* D\chi \quad (3)$$

where:

$$\begin{aligned} S_b[\phi, \chi] = a^D \sum_x b \sum_{n=0}^{N-1} & \left[-b^{-2} (\phi_{n+1}^*(x) \phi_n(x) + h.c. - 2\phi_n^*(x) \phi_n(x)) + \right. \\ & + b^{-1} (\imath \phi_{n+1}^*(x) B \phi_n(x) + h.c.) + \frac{1}{2} (\phi_{n+1}^*(x) B^2 \phi_n(x) + h.c.) + \\ & \left. + \sqrt{L} \exp\{-mbn\} (\chi^*(x) (m + \imath B) \phi_n(x) + h.c.) \right] + \frac{a^D L}{2m} \sum_x \chi^*(x) \chi(x) \end{aligned} \quad (4)$$

and the free boundary conditions in t are imposed:

$$\phi_n = 0 ; n < 0 ; n \geq N \quad (5)$$

The bozonic D-dimensional fields $\chi(x)$ have the same spinorial and internal structure as the fields $\psi(x)$.

The bozonic action (4) is a linearized version of the expression in the exponent of the following integral:

$$\begin{aligned} I = \int \exp \left\{ a^D \sum_{\alpha} b \sum_{n=0}^{N-1} \left[b^{-2} (\phi_{n+1}^{\alpha*} \exp\{-\imath B_{\alpha} b\} \phi_n^{\alpha} + h.c. - 2\phi_n^{\alpha*} \phi_n^{\alpha}) - \right. \right. \\ \left. \left. - \sqrt{L} \exp\{-mbn\} (\chi^{\alpha*} (m + \imath B_{\alpha}) \phi_n^{\alpha} + h.c.) \right] - \frac{a^D L}{2m} \sum_{\alpha} \chi^{\alpha*} \chi^{\alpha} \right\} D\phi^* D\phi D\chi^* D\chi \end{aligned} \quad (6)$$

where instead of x -representation we used a basis formed by the eigenvectors of the operator B , B_{α} being corresponding eigenvalues.

Indeed, taking into account that $b \parallel B \parallel \ll 1$, we can expand the expression in the exponent of the integrand (6) in a Taylor series. Keeping only the terms, nonvanishing in the limit $b \rightarrow 0$, we get the expression (4). For a finite b the difference between (3) and (6) is of order $O(b^2 \parallel B \parallel^2)$.

By changing variables

$$\phi_n^{\alpha} \rightarrow \exp\{-\imath B_{\alpha} nb\} \phi_n^{\alpha} ; \phi_n^{\alpha*} \rightarrow \exp\{\imath B_{\alpha} nb\} \phi_n^{\alpha*} \quad (7)$$

we can rewrite the eq. (6) as the gaussian integral over ϕ with the quadratic form which does not depend on B_α . To calculate this integral it is sufficient to find a stationary point of the exponent.

For small b the sum over n can be replaced by the integral and the equations for the stationary point acquire the form:

$$\ddot{\phi}^\alpha - \sqrt{L}\chi^\alpha(m - \imath B_\alpha)e^{-(m-\imath B_\alpha)t} = 0 \quad (8)$$

$$\phi^\alpha(0) = \phi^\alpha(L) = 0 \quad (9)$$

(One can show that replacing the sum by the integral also introduces corrections of order $O(b^2 \parallel B \parallel^2)$.)

The solution of these equations is:

$$\phi^\alpha(t) = \frac{\chi^\alpha \sqrt{L}}{m - \imath B_\alpha} \left(e^{-(m-\imath B_\alpha)t} + \frac{t}{L} (1 - e^{-(m-\imath B_\alpha)L}) - 1 \right) \quad (10)$$

Substituting these solutions to the integrand ,we get:

$$\lim_{b \rightarrow 0} I = \int \exp \left\{ - \sum_\alpha \frac{\chi^{\alpha*} \chi^\alpha}{m^2 + B_\alpha^2} (1 - 2e^{-mL} \cos B_\alpha L + e^{-2mL}) \right\} D\chi^* D\chi \quad (11)$$

Therefore

$$\lim_{b \rightarrow 0, L \rightarrow \infty} I = \det(B^2 + m^2) \quad (12)$$

The equality (3) is proven. For finite b and L this equation has to be corrected by the terms:

$$O(b^2 \parallel B \parallel^2) + O(e^{-mL}) \quad (13)$$

In the next section we apply this construction to simulations of a one dimensional model.

3 Numerical simulations for free fermions on the 9^1 lattice.

Some technical issues of the new algorithm can be observed by performing numerical simulations on 1D lattice for free fermions. We used the following action:

$$S_f = \sum_k \psi_k^* (-\partial^2 + m^2) \psi_k \quad (14)$$

where ψ^*, ψ are anticommuting Grassman variables, ∂ is symmetrical lattice derivative and m is a mass. The lattice spacing a has been set equal to 1 for convenience. One can rewrite the operator in the quadratic form of (14) as follows:

$$-\partial^2 + m^2 = B^2 + m^2 \quad (15)$$

where $B = (\imath\partial)$ is hermitian matrix. So in accordance with the discussion above the path integral over Grassmanian variables ψ^*, ψ can be approximated by the path integral over bozonic fields ϕ, χ . The corresponding bozonic theory with the multiquadratic action $S_b[\phi, \chi]$ (see eq.(4)) can be simulated straightforwardly using local heatbath and overrelaxation algorithms.

We note that for the model (14) the action $S_b[\phi, \chi]$ can be rewritten in the form:

$$S_b[\phi, \chi] = \tilde{S}[\rho, \beta] + \tilde{S}[\sigma, \gamma] \quad (16)$$

where ρ, β and σ, γ are real and imaginary parts of the fields ϕ, χ :

$$\begin{aligned} \phi &= \rho + i\sigma \\ \chi &= \beta + i\gamma \end{aligned} \quad (17)$$

Hence the path integral over the fields ϕ, χ allows the following factorization:

$$\mathcal{Z}_b = \int e^{-S_b[\phi, \chi]} D\phi^* D\phi D\chi^* D\chi = \left[\int e^{-\tilde{S}[\rho, \beta]} D\rho D\beta \right]^2 \quad (18)$$

It makes possible to simulate the theory with the real fields ρ, β and the action $\tilde{S}[\rho, \beta]$, accelerating the calculations by the factor of 2. The resulting partition function must be squared.

Let us firstly consider the updating of the field ρ . If all field variables except ρ at point (x, t) are kept fixed (where t numerates points in auxiliary dimension), the action assumes the following form:

$$S_b[\rho(x, t)] = A(\rho(x, t) - E(x, t))^2 + \text{const} \quad (19)$$

where A is a positive constant and $E(x, t)$ is an easily calculable vector. A local update

$$\rho(x, t) \rightarrow \tilde{\rho}(x, t) = \omega E(x, t) + (1 - \omega)\rho(x, t) + \sqrt{\frac{\omega(2 - \omega)}{A}}\eta \quad (20)$$

where η is a gaussian random number of unit variance, fulfills detailed balance for any $0 < \omega \leq 2$ [7].

In our test we used hybrid overrelaxation algorithm, which consists in the mixing of heatbath ($\omega = 1$) and overrelaxation ($\omega = 2$) sweeps with a ratio $1 : N_{or}$ [8]. It is believed that this algorithm has a dynamical critical exponent $z \approx 1$ if N_{or} is proportional to the correlation length ξ .

Generally we subdivided the lattice into 2 sublattices, coloring each site according to the function

$$C(x, t) = (-1)^t$$

One can see that $E(x, t)$ does not depend on the field variables at the same t and sites of the same colour do not interact with each other. We updated one colour after the other.

Analogously, if all field variables except β at point x are fixed, the action assumes the form:

$$S_b[\beta(x)] = C(\beta(x) - D(x))^2 + \text{const} \quad (21)$$

where C is a positive constant. Since field β is interacting with $\rho(x, t)$ for all t , the computation of the vector $D(x)$ requires an effort proportional to N , i.e. a β field update is almost as expensive as the updating of ρ field.

In our implementation, the iteration is made up of one ρ heatbath sweep, N_{or}^ρ overrelaxation sweeps, one β heatbath sweep and N_{or}^β overrelaxation sweeps. After each iteration the following function was measured:

$$\mathcal{R} = \left\langle \sum_k \psi_k \psi_k^* \right\rangle \quad (22)$$

To measure the function (22) using the bozonic approximation of the fermionic theory with the action (14), one must rewrite (22) as a correlation function of ρ, β fields with the measure defined by $\tilde{S}[\rho, \beta]$. Let us denote:

$$Z_f = \int e^{-S_f} D\psi^* D\psi \quad (23)$$

$$Z_b = \int e^{-\tilde{S}[\rho, \beta]} D\rho D\beta \quad (24)$$

In the section 2 it was proved that

$$Z_f = Z_b^2 + O(b^2 \|B\|^2) + O(e^{-mL}) \quad (25)$$

Then we can derive:

$$\mathcal{R} = \frac{1}{2mZ_f} \frac{\delta}{\delta m} Z_f \approx \frac{1}{2mZ_b^2} \frac{\delta}{\delta m} Z_b^2 = \frac{1}{mZ_b} \frac{\delta}{\delta m} Z_b = -\frac{1}{m} \left\langle \frac{\delta \tilde{S}[\rho, \beta]}{\delta m} \right\rangle_{\rho, \beta} \quad (26)$$

and

$$\mathcal{R}_b = -\frac{1}{m} \left\langle \frac{\delta \tilde{S}[\rho, \beta]}{\delta m} \right\rangle_{\rho, \beta} \quad (27)$$

We used the expression (27) as a bozonic approximation to the function (22). One can see that the accuracy of this approximation is also given by the expression (13).

In table 1 the autocorrelation time dependence is displayed for several updating schemes. Autocorrelation times were measured for the function (27) using the method proposed by Socal [9], namely

$$\tau_{int}(\mathcal{R}_b) = \frac{1}{2} + \sum_{i=1}^M \frac{C(i)}{C(0)} \quad (28)$$

with

$$C(i) = \frac{1}{n-i} \sum_{k=1}^{n-i} (\mathcal{R}_k - \overline{\mathcal{R}})(\mathcal{R}_{k+i} - \overline{\mathcal{R}}) \quad (29)$$

where the n is a number of iterations and M chosen so that $\tau_{int} \ll M \ll n$. An estimate for the error of τ_{int} is given by

$$\sigma_{\tau_{int}}^2 = \frac{2(2M+1)}{n} \tau_{int}^2 \quad (30)$$

One can see that overrelaxing β field does not decrease autocorrelation time substantially (it even may increase τ_{int} in units of CPU time). Contrary, overrelaxing ρ field improves the autocorrelation behavior. When adding more overrelaxation sweeps for the given sets of parameters, τ_{int} in CPU units starts to rise again.

Updating	\mathcal{R}_b	$\tau_{int}(\mathcal{R}_b)$
Hh	0.526(10)	56(11)
HOh	0.534(7)	20(3)
HhOo	0.544(9)	22(4)
HOhO	0.546(6)	10(1)
HOhOo	0.546(6)	9(1)
HOhOO	0.544(4)	4.3(3)
HOOhOO	0.543(3)	2.8(2)
HOOOhOO	0.541(3)	2.2(2)
HOOhOOOo	0.541(2)	1.6(1)

Table 1: Autocorrelation times in [1/iteration] units on 9^1 lattice for $m = 4, N = 100$ and $b = 0.015$. The letters in the first column give the type and order of sweeps used per iteration, where H is a ρ heatbath, O is a ρ overrelaxation and h and o are the β updates. The exact value of \mathcal{R} is 0.5457.

Now we discuss the systematic error and autocorrelation behavior of the algorithm. We measure the function \mathcal{R}_b (see (27)) and $\tau_{int}(\mathcal{R}_b)$ for different sets of parameters b and N . As it is demonstrated in section 2, the systematic error is given by:

$$\Delta = \Delta_1 + \Delta_2, \quad (31)$$

where:

$$\Delta_1 = Cb^2 + Fb^3 + O(b^4), \quad (32)$$

$$\Delta_2 = De^{-mbN}, \quad (33)$$

and C, F, D are some constants.

To control the systematic error one can fix the parameter mbN and perform calculations for different values of b . We choose $m = 4$, $mbN = 8$. The results are shown on Fig.1 where the function $\mathcal{R}_b(mb)$ (27) is plotted (the statistical errors are small). The horizontal line corresponds to the theoretical value (22). It is seen that the results converge to the theoretical value as mb decreases. The fit of expression (32) for Δ_1 gives $C \approx 17$ and $F \approx -43$. The systematic error $O(b^2)$ is partially compensated by the $O(b^3)$ error.

On Fig.2 the dependence of the autocorrelation time for \mathcal{R}_b against mb is plotted. In these and all further measurements HOhOO scheme is used. From these data we get that $\tau_{int}(\mathcal{R}_b) \approx 0.25/mb$ when $mb \rightarrow 0$.

Now let us fix the parameter $b = 0.01$ making Δ_1 less than 0.002 and measure \mathcal{R}_b and $\tau_{int}(\mathcal{R}_b)$ for the different number of points in auxiliary dimension N . On Fig.3 the dependence of \mathcal{R}_b against N is shown. The horizontal line denotes the theoretical value of (22). From these data we get $D < 2.5$.

On Fig.4 the dependence of $\tau_{int}(\mathcal{R}_b)$ against N is plotted. The autocorrelation time grows quadratically when N increases, but the proportionality factor is very small: $\sim 10^{-4}$. For large N the autocorrelation time can be decreased by adding more overrelaxation sweeps of the ρ field. To investigate the autocorrelation behavior of the algorithm for the cases of practical importance one needs to study the models of larger dimensionality with the gauge fields involved.

In conclusion we investigate the slowing down of the algorithm at small values of m . We fix $b = 0.015$ and $mbN = 6$ making the systematical error constant. The results are shown on Fig.5, the fit of these data gives $\tau_{int}(\mathcal{R}_b) \approx \frac{C}{m^\alpha}$, $C \approx 3.3$, $\alpha \approx 2$.

4 Discussion.

We performed the first simulations for Slavnov's algorithm on 1D lattice for free fermions. It was shown that correct and accurate results can be obtained with a reasonable size of lattice in auxiliary dimension. We are going to extend this simulations to larger lattices taking into account interaction with the gauge fields (in progress).

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FIG.1

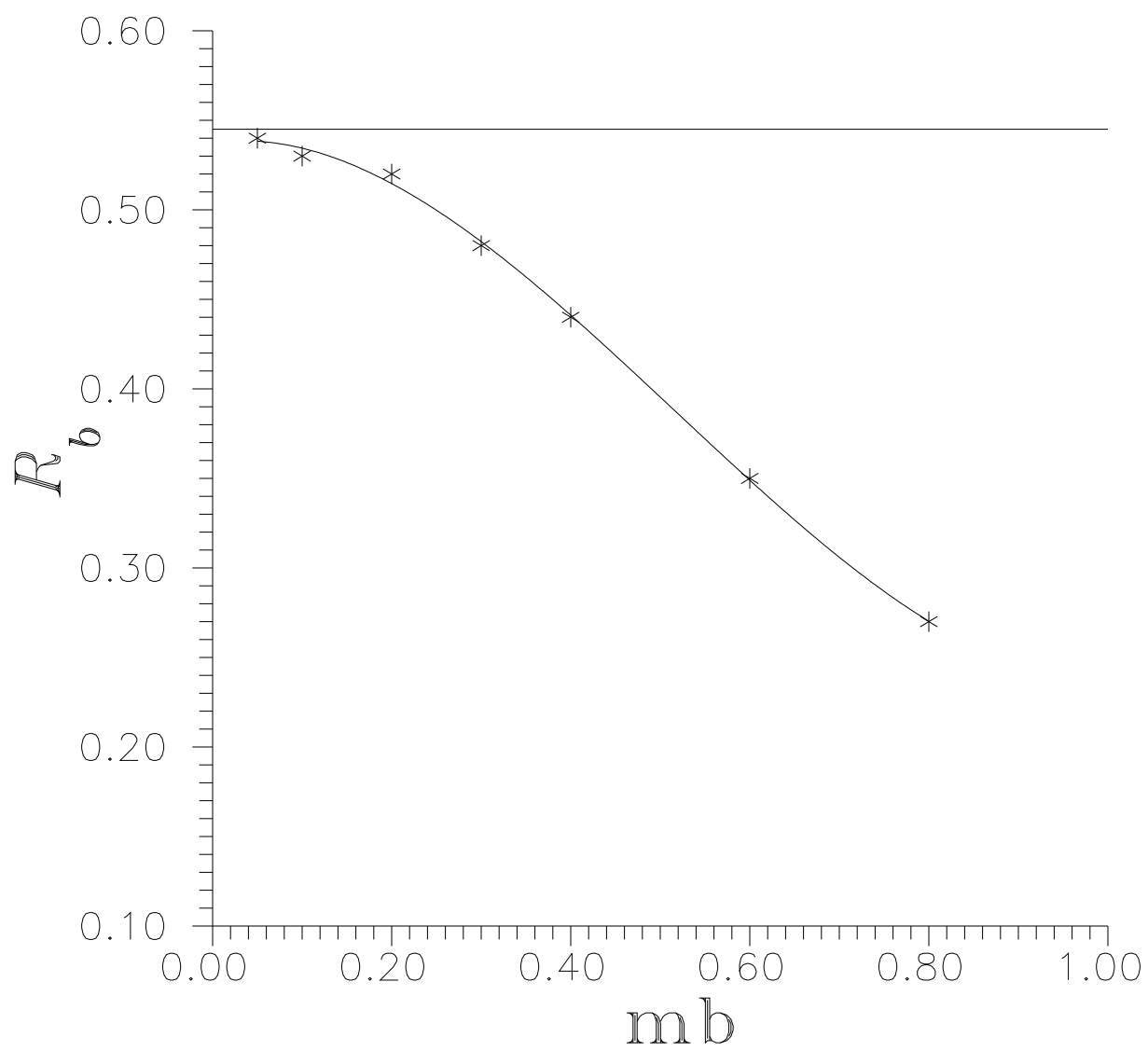


FIG.2

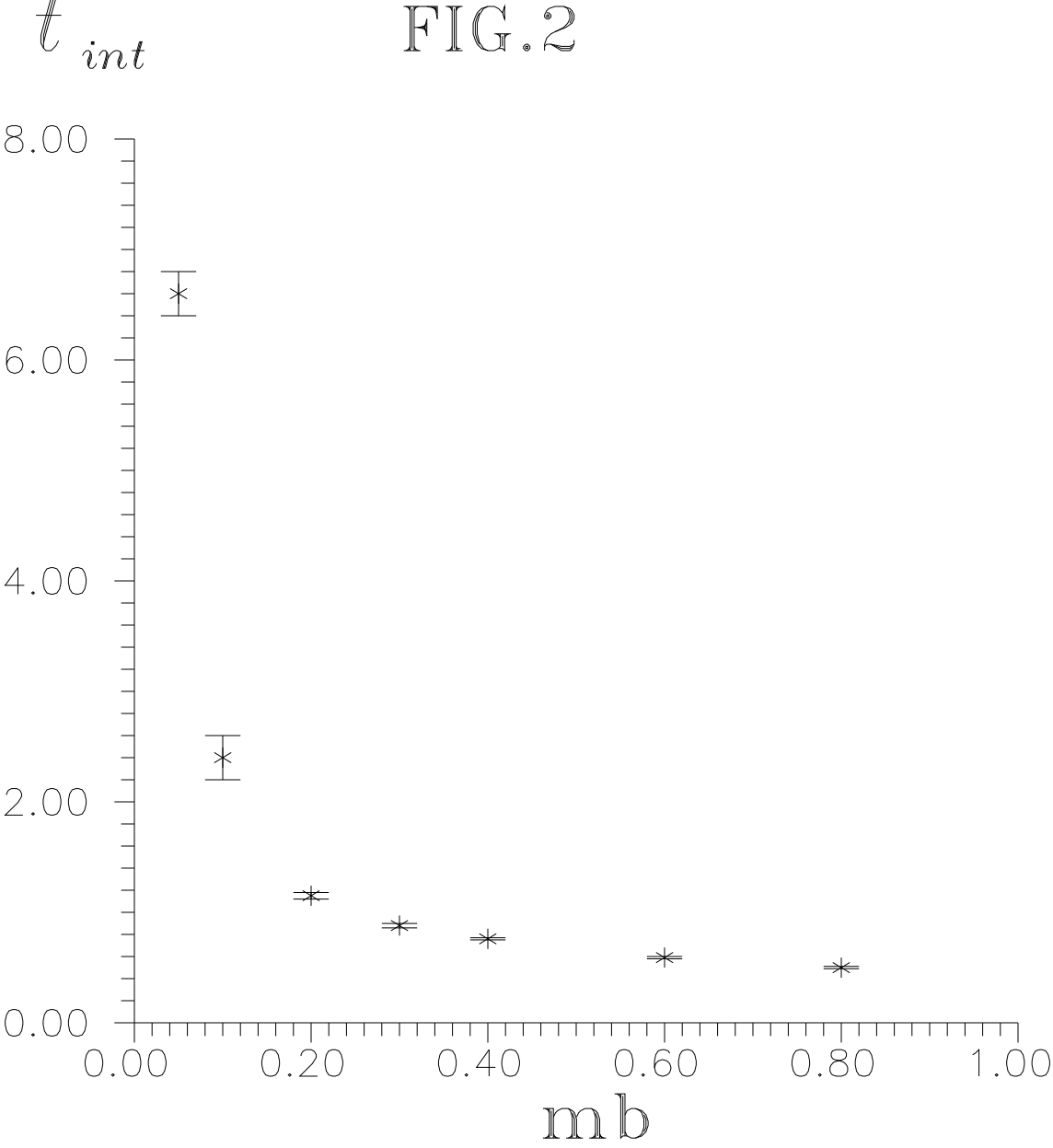


FIG.3

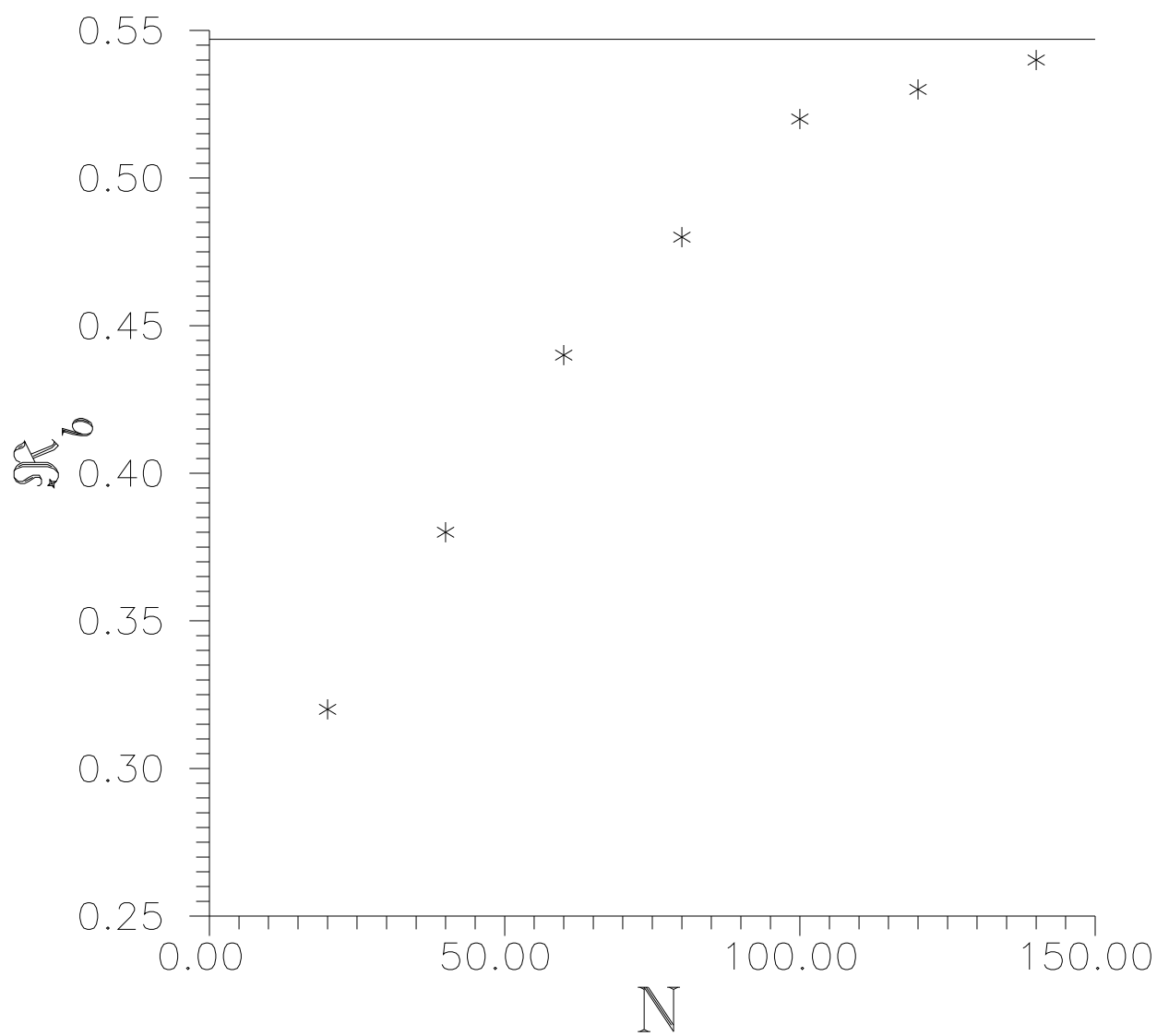


FIG.4

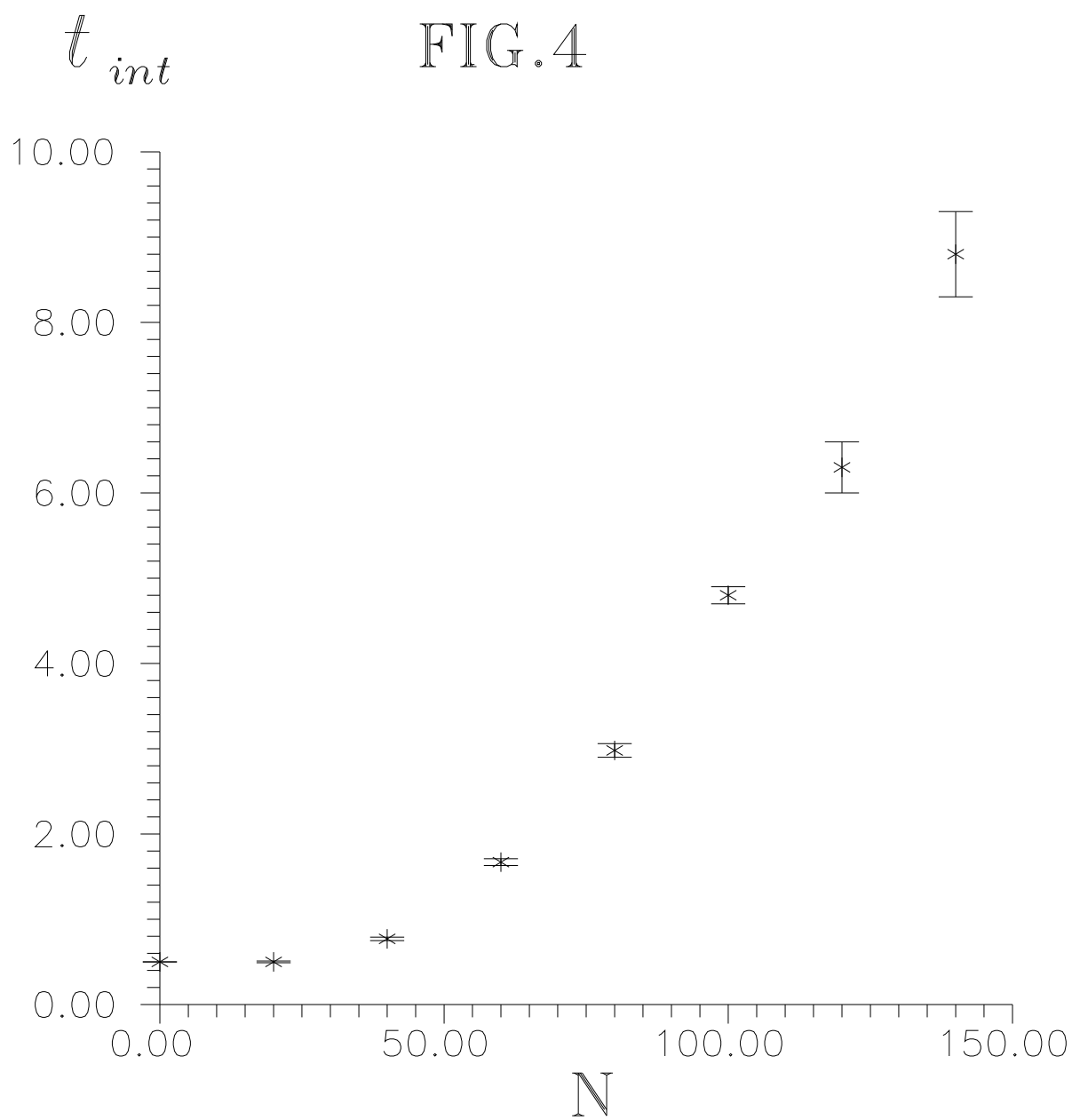


FIG.5

